Unit 1: Atomic Structure

1.1 Particles in the atom and atomic radius

Atoms: mostly empty space surrounding a very small, dense nucleus that contains protons and neutrons, electrons are found in shells in the empty space around the nucleus

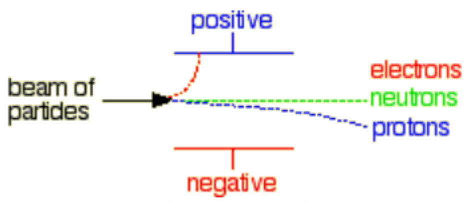
Particle	**neutron**	**proton**	**Electron**
Charge/e	0	+1	-1
Mass/au	1	1	$\frac{1}{1840}$

Atomic number/proton number: number of protons in the nucleus of an atom, the same for all atoms of the same elements
Mass number/nucleon number: total number of protons AND neutrons in the nucleus of an atom, may be different due to isotopes

Distribution of mass and charge within an atom:
The mass of an atom is almost all concentrated in the nucleus as the mass of the electrons is negligible compared to the mass of protons and neutrons
The nucleus is positively charged and an electrically neutral atom, there is the same number of protons and electrons

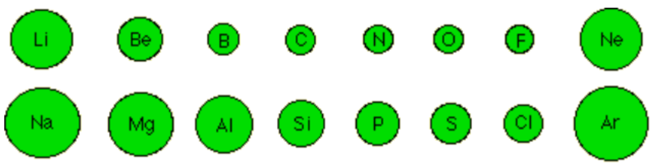
Movement of beams of the atomic particles in an electric field, moving at the same velocity:

Protons are deflected on a curved path towards the negative plate
Electrons are deflected on a curved path towards the positive plate
Neutrons continue in a straight line



The lighter electrons however, are deflected far more strongly than the heavier protons as they have a lower inertia

Atomic Radius:
Across a period, the atomic radius decreases as the nuclear charge increases as well as the number of electrons increases causing a greater attractive force between the outer electrons and the nucleus
Down a group, the atomic radius increases as more layers of electrons are added



Ionic Radius:
Across a period, the trend can be divided into the positive ions and negative ions, all ions in the same group are isoelectronic
In the positive ions, they are smaller than their atoms as a layer of electrons is lost, the ionic radius decreases as across the group the number of protons increases so there is a greater pull
In the negative ions, they are larger than their atoms as there Is an additional layer of electrons, the ionic radius decreases as the proton number increases and so does the attraction of the nucleus for the outer electrons

Down a group, the ionic radius increases as more layers of electrons/shells

1.2 isotopes

Isotopes are atoms of the same element with the same atomic number but a different mass number/number of neutrons
They have the same **chemical properties** as they have the same configuration and number of electrons in the outermost shell
They have different **physical properties** as they have different masses and densities which are dependent on the mass number

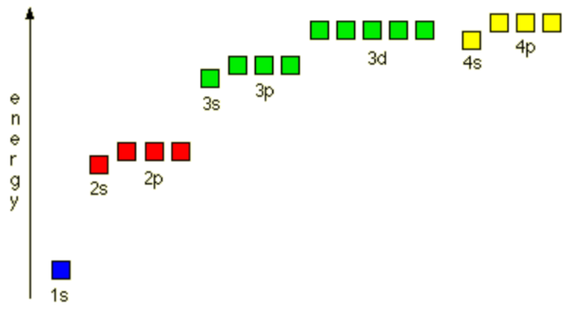
Isotonic atoms have the same number of neutrons
radioisotopes are isotopes that have an unstable nucleus and may emit nuclear radiation

$^{X}A_{Y}$ where x is the mass number and y is the atomic number

1.3 Electrons, energy levels and atomic orbitals

Shell: specific distances associated energy from the nucleus where electrons are found with particular energies
Sub-shell: specific distances associated with a specific energy where electrons are found (in sub units of shells)
Orbital: places where electrons are found within a subshell (Each orbital holds 2 electrons maximum)
Principal quantum number: amount of energy in specific distances from shells
Ground state: most stable electronic configuration of an atom & the energy level of an atom with the least energy of all possible states

There are three types of orbitals/sub shells: *s*, *p*, and *d* each can carry a maximum number of electrons
s sub shells can carry 2 electrons as it has 1 orbital
p sub shells can carry 6 electrons as it has 3 orbitals
d sub shells can carry 10 electrons as it has 5 orbitals



Each shell only has a specific number of sub shells:
Shell 1 has *s* subshell only
Shell 2 has *s* and *p* subshells
Shell 3 has *s p* and *d* sub shells
Shell 3 has *s p d* and *f* subshells

Total number of orbitals in a shell: n^2
Total number of electrons in a shell: $2n^2$

Within the first three subshells, the order of energy increases making the 1s subshell carrying the least amount of energy

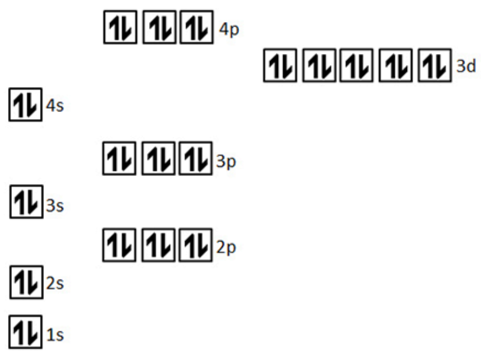
The periodic table can be split up into "blocks" the first 2 groups are "s block" the transition elements are the "d" block and the non-metals are the "p block" each block respectively states what subshell the elements in that block have as their highest energy level

Heisenberg's uncertainty principle states that the momentum and position of an electron cannot be determined together
The Aufbau Principle states that Electrons fill low energy orbitals (closer to the nucleus) before they fill higher energy ones.
Hund's rule states that every orbital in a subshell is singly occupied with one electron before any one orbital is doubly occupied, and all electrons in singly occupied orbitals have the same spin.
Pauli exclusion principle states that no more than 2 electrons can fill a single orbital, and that if two electrons occupy it, one goes "up" and one goes "down" meaning that they spin in opposite directions

Exceptions to these principles and rules: chromium and copper
Rather than filling $4s^2$ before $3d^5$ and $3d^{10}$ respectively only $4s^1$ is filled

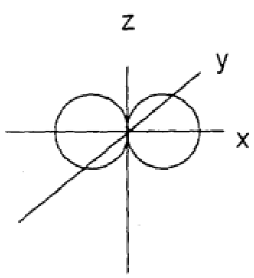
Krypton electronic configuration: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6$

Krypton's electrons in box notation:

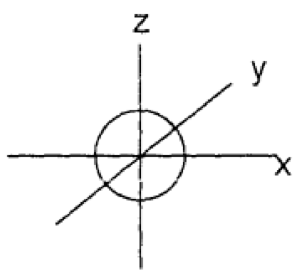


Free radical: a species with one or more unpaired electron

Shape of a *p* orbital:



Shape of an *s* orbital:



1.4 ionization energy:

First ionization energy: the energy required to remove one mole of the most loosely held electron from one mole of gaseous atoms to produce 1 mole of gaseous ions with a charge of +1.
It's measured in kilojoules per mole and varies from 381-2370.
It is due to the attraction between the nucleus and the outermost electron

$$X(g) \longrightarrow X^+(g) + e^-$$

It shows periodicity as it varies in repetitive across the periodic table and provides proof for shells and subshells in atom

Factors influencing first ionizations energy include:

Nuclear charge, as the more protons there are in the nucleus, the more positively charged it is, and the more strongly the electrons are attracted to it, so the more energy is required to remove the electron
Distance of the electrons from the nucleus, as attraction falls off very rapidly with distance, an electron closer to the nucleus will be much more strongly attracted than one further away, so the bigger the atom, the easier it is to remove electrons
The number of electrons between the outer electrons and the nucleus, the layers of electrons between the outer electrons and nucleus lessens the pull of the nucleus and this is known as electron shielding, the more electron shells present, the less energy is required to remove an electron
Whether the electron is on its own in an orbital or is paired with another electron, as two electrons in the same orbital experience a bit of repulsion from each other which offsets the attraction of the nucleus making it more easily removed, this is known as spin-pair repulsion, if it is present, the less energy is required to remove an atom

Trend in first ionizations energies:

Across a period, they increase across a period as the nuclear charge increases causing a greater force of attraction between the nucleus and the electrons so more energy is required. As they are all in the same shell, electron shielding is the same but the distance from the nucleus is almost the same but across the period, the atomic radius slightly decreases which takes part

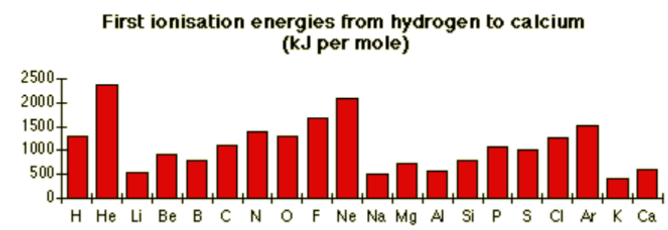
There is however an exception which is the drop between the elements in group 2 and 3 (Be and B & Mg and Al) this is because the electrons are now filling up the 2p/3p orbital rather than the 2s/3s orbitals which have a slightly higher energy and can be found relatively further away from the nucleus, this increased distance results in a reduced attraction AND the p orbitals are not only experiencing electron shielding from the prior shells but also the prior and respective s subshell, which decreases the first ionizations energy

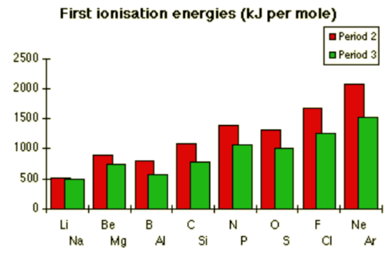
There is again an exception which is the drop between the elements in group 5 and 6 (N and O & P and S), they share the same electron shielding as they are both in the 2p/3p orbitals but the difference is that in the element in group 6, the electron is being removed from an orbital that is now filled with 2 electrons, meaning that the repulsion between these two electrons decreases the first ionizations energy

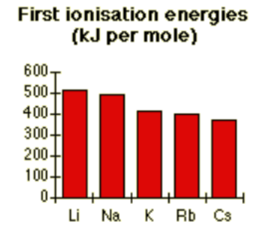
Down a group, they decrease as although the nuclear charge is greater but the greater atomic radius causes a greater nuclear distance and electron shielding offsets this change. Electrons in the same group are also in the same orbital and subshell type

Successive ionizations energy: It is the energy needed to remove x electron from each ion in 1 mole of gaseous (x-1)+ ions to give x+ ions.

It can be used to work out which group an element is in, because there will be a large jump when suddenly breaking into an inner level, smaller odd jumps can also be caused by the aforementioned exceptions
Successive ionizations energies get larger as you go on as you are left with a positive ion and removing an electron from an already positive ion is harder than from an atom, as well as when you progressively go on







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